A review of flux identification methods for models of sedimentation

R. Bürger, J. Careaga and S. Diehl

ABSTRACT

Most models of sedimentation contain the nonlinear hindered-settling flux function. If one assumes ideal conditions and no compression, then there exist several theoretically possible ways of identifying a large portion of the flux function from only one experiment by means of formulas derived from the theory of solutions of partial differential equations. Previously used identification methods and recently published such, which are based on utilizing conical vessels or centrifuges, are reviewed and compared with synthetic data (simulated experiments). This means that the identification methods are evaluated from a theoretical viewpoint without experimental errors or difficulties. The main contribution of the recent methods reviewed is that they, in theory, can identify a large portion of the flux function from a single experiment, in contrast to the traditional method that provides one point on the flux curve from each test. The new methods lay the foundation of rapid flux identification; however, experimental procedures need to be elaborated.

Key words | batch flux function, calibration, hindered settling, identification, inverse problem, partial differential equation

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INTRODUCTION

The hindered-settling batch flux function is defined by $f(C) = Cv_{\mathrm{hs}}(C)$, where C is the concentration and $v_{\mathrm{hs}}(C)$ is the hindered-settling velocity. This function is a key ingredient in models of clarifier-thickeners and it is therefore unavoidable to identify $f(C)$ for the suspension under study. Calibration usually means finding parameter values within a *given* functional expression (e.g. Vesilind or Takács exponential functions). Sometimes it is not obvious which functional expression to choose. This problem arises, in particular, for activated sludge (Li & Stenstrom 2014; Torfs *et al.* 2017). Then the entire flux function is the unknown. The so-called inverse problem to identify a function in a model equation given part of its solution (in practice, real data) is in general difficult and often ill-posed; two different flux functions can give the same batch test solution for a given initial concentration.

To illustrate the latter statement of ill-posedness, we consider a standard batch test with the initial concentration $C_0 = 2$ g/l, where the flux function $f(C)$ is increasing. The dynamic solution consists for a while of the concentration 2 g/l below the sludge blanket level (SBL) and in the waves from the bottom there is an interval of high concentrations, say 10 g/l and higher. Since the concentrations between 2 and 10 g/l are not present in the solution, the flux function can be changed in that interval. The same holds for concentrations less than 2 g/l. This also illustrates that a constitutive function can only be identified for those concentrations, or a part of them, that are present in the solution (in practice, the real data available). Consequently, either one has to repeat a simple experiment many times (e.g. the traditional batch-settling test with different initial concentrations), or one has to find another experiment in which a range of concentrations appear, preferably a large interval. We review here a couple of published experiments that satisfy the latter, which we may denote a 'rich experiment'.

In addition to having a rich experiment, another requirement for obtaining a successful solution of the inverse problem, is to at least have formulas for the graph of the flux function $f(C)$, or parts of it, expressed by measurable variables such as the location of the SBL as function of time. Rich experiments have been suggested and such formulas derived from the theory of solutions of partial differential equations (PDEs) (Diehl 2007; Bürger & Diehl 2013; Bürger *et al.* 2018a, 2018b; Careaga & Diehl 2020).

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Although many factors influence a sedimentation process, such as compression at high concentrations, the distribution of particle size and density, flocculation and breakage processes, the main nonlinearity of the process that leads to discontinuities in the concentration profile can be captured by a PDE that only involves $f(C)$. The next phenomenon to include is compression above a certain critical concentration. Then the model is a degenerate parabolic PDE (Bürger *et al.* 2005, 2011, 2013), which has been widely accepted for the one-dimensional simulation of settling tanks (Li & Stenstrom 2014; Torfs *et al.* 2015; Baalbaki *et al.* 2017; Saagi *et al.* 2017; Tonge *et al.* 2019). The constitutive assumption for compression is an effective solids stress function, which appears as another term in the model PDE and has a smoothing effect on the concentration profile above the critical concentration. The effective solids stress function can in principle be identified by measuring the steady-state concentration profile of a batch test in a cylindrical vessel or from accurate data of batch tests (De Clercq 2006; Diehl 2015). Empirical methods (PDE theory is not used) for flux identification when compression is present have been suggested by e.g. Bueno *et al.* (1990), Font & Laveda (2000) and Stricker *et al.* (2007). PDE-based methods for the simultaneous identification of both the flux and the effective solids stress function have been presented by Coronel *et al.* (2003), De Clercq (2006), Bürger *et al.* (2009) and Diehl (2015). However, the inverse problem is ill-posed and the methods of identification are complicated.

The purpose of this contribution is to review methods for the identification of the hindered-settling flux function, either when there is no compression, or up to the critical concentration. Recent publications have shown that one can then utilize results for hyperbolic PDEs to obtain formulas for parts of the flux function without assuming any particular functional expression (exponential, power law, polynomial, etc.) (Diehl 2007; Bürger & Diehl 2013; Bürger *et al.* 2018a, 2018b; Careaga & Diehl 2020). The methods are demonstrated on synthetic data with low noise; that is, simulated experiments from which data are taken. Thereby, the inherent properties of the methods can be investigated and compared without the additional difficulties associated with experiments with real suspensions.

While we here review flux identification methods for sedimentation, we mention that some other PDE-based methods have been published; see a short review by Bürger *et al.* (2018a). We do not include those methods here since we assess that they are less suitable for the sedimentation problem, but may be successful in other applications, such as traffic flow (Holden *et al.* 2014).

A related inverse problem for the sedimentation of a polydisperse suspension (which consists of particles of different settling velocities) is to identify the mass distribution with respect to different settling velocities. Chancelier *et al.* (1998) introduced several measurement procedures and showed how the mass distribution can be estimated under the assumption that the settling velocity of a particle is constant, so that the flux is linear. This is reasonable for low concentrations only and therefore appropriate for primary settling tanks or the effluent of secondary settling tanks. The theoretical findings by Chancelier *et al.* (1998) were used by Chebbo & Gromaire (2009), who developed the VICAS protocol to be used by plant operators.

ASSUMPTIONS AND SYNTHETIC DATA

We model batch sedimentation by gravity in a closed vessel by the conservation PDE

$$\frac{\partial(A(z)C)}{\partial t} - \frac{\partial(A(z)f(C))}{\partial z} = 0, \qquad 0 < z < H,$$

where $C = C(z, t)$ is the solids concentration at height z, measured from the bottom of the vessel, and time t, and $A(z)$ is the cross-sectional area, which may vary with z.

Synthetic data are produced by simulations of several types of batch tests and with the following flux function (Diehl 2015); see the dashed graph in the figures:

$$f(C) = \frac{Cv_0}{1 + (C/\bar{C})^q} - \frac{Cv_0}{1 + (C_{\max}/\bar{C})^q},$$
$$v_0 = 10^{-3}\ \mathrm{m/s},\ \ \bar{C} = 4\ \mathrm{kg/m^3},\ \ q = 3,$$

where the term with the maximum concentration $C_{\max} = 20\ \mathrm{kg/m^3}$ is added to ensure that $f(C_{\max}) = 0$ (the flux must be zero at a finite concentration when compression is not modelled). A common assumption is that the flux function has one inflection point; here, it is $C_{\mathrm{infl}} = 6.5\ \mathrm{kg/m^3}$. The simulations are made with established numerical methods; see Bürger *et al.* (2018a) and references therein.

Several of the flux identification methods below use that the descending SBL $z = h(t)$ in a batch test is known so that its velocity $h'(t)$ can be computed. The function $h(t)$ can be obtained by fitting piecewise cubic polynomials with the least-squares method with constraints to observations of the position of the SBL at discrete times; see Supplementary

Material. Various devices for automatic detection of the SBL have been developed; see François et al. (2016), Derlon et al. (2017) and references therein.

FLUX IDENTIFICATION METHODS WITH ADVANTAGES AND DISADVANTAGES

We now state some methods of flux identification and comment on advantages and disadvantages, and refer to the mentioned publications for the derivation of the formulas that give the flux function $f(C)$. In some cases $f(C)$ can be given by an explicit formula; however, it contains sums of several functions defined on smaller intervals. We present here only parameterized formulas that pair an expression for the concentration C in terms of $h(t)$ and $h'(t)$ with the corresponding value of the flux $f(C)$. The cross-sectional area $A(z)$ is constant in Methods 1–4.

Method 1. Traditional batch-settling test: An initially homogeneous suspension of concentration C_0 settles and $h'(t)$ is recorded; see Figure 1. Except for a possible initial induction period, the settling velocity is constant until waves from the bottom reach the SBL. This gives one point on the flux curve (Vanderhasselt & Vanrolleghem 2000; Torfs et al. 2016; Derlon et al. 2017). The method is simple but time consuming unless several experiments can be conducted simultaneously; for example, with the five-column SediRack device (Concha 2014).

Method 2. Kynch test (KT) with tail identification: One obtains $h(t)$ and $h'(t)$ from a traditional batch test; see Figure 1. In addition to the information from Method 1, it is possible to estimate a part of the flux above the inflection point (the tail). This is the graphical method by Kynch (1952), which has been elaborated by, among others, Lester et al. (2005) and was eventually described by the following parametric formula (Diehl 2007):

$$(C, f(C)) = \frac{HC_0}{h(t) - th'(t)}(1, \ -h'(t)), \qquad t_{\text{start}} \le t \le t_{\text{end}}, \quad (1)$$

where the time interval is the curved part of the SBL; see Figure 2. The advantage of this method is that the tail of the flux is identified from only one batch test.

Method 3. Diehl test (DT): A batch test where initially a layer of high concentration C_0 (for $0 < H_0 < z < H$) is placed on top of clear water (for $0 < z < H_0$) separated by a membrane that bursts at the start; see Figure 1. A part of the flux to the left of the inflection point can be identified by the parametric formula (Diehl 2007)

$$(C, f(C)) = \frac{(H - H_0)C_0}{h(t) - th'(t) - H_0}(1, \ -h'(t)), \quad t_{\text{start}} \le t \le t_{\text{end}}, \quad (2)$$

where the time interval corresponds to the concave part of the SBL; see Figure 2. A theoretical advantage is that part of the flux below the inflection point can be identified from one test. A disadvantage is that special equipment is needed and it is difficult to start under ideal conditions without turbulence.

Method 4. Identification with finite elements (Figure 3): Many data points are required in both time and height (KT or DT) also below the SBL; see the non-invasive measurements by De Clercq (2006). The flux function can be identified as a linear combination of continuous finite-element hat functions by solving a linear system of

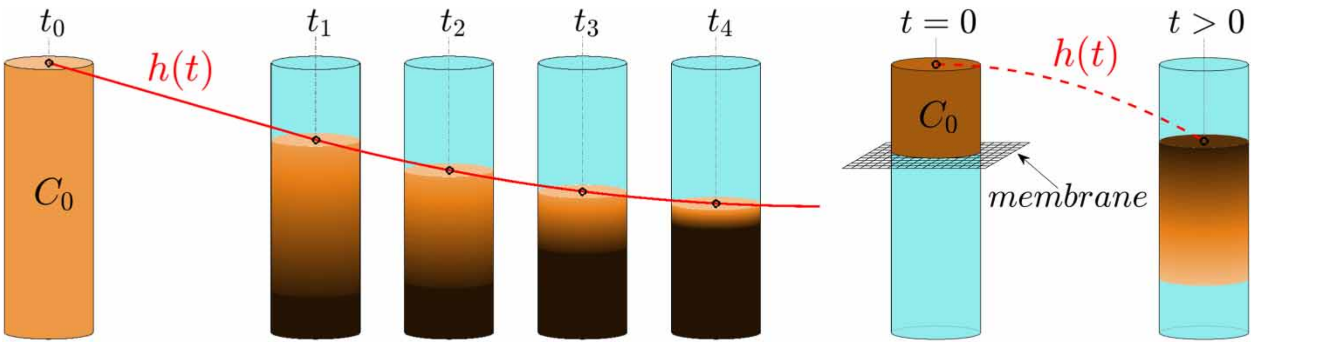

Figure 1 | Left: A traditional batch-settling test, or a Kynch test (KT), in a cylinder with constant cross-sectional area. Right: A Diehl test (DT) with initially a layer of high concentration on top of clear water.

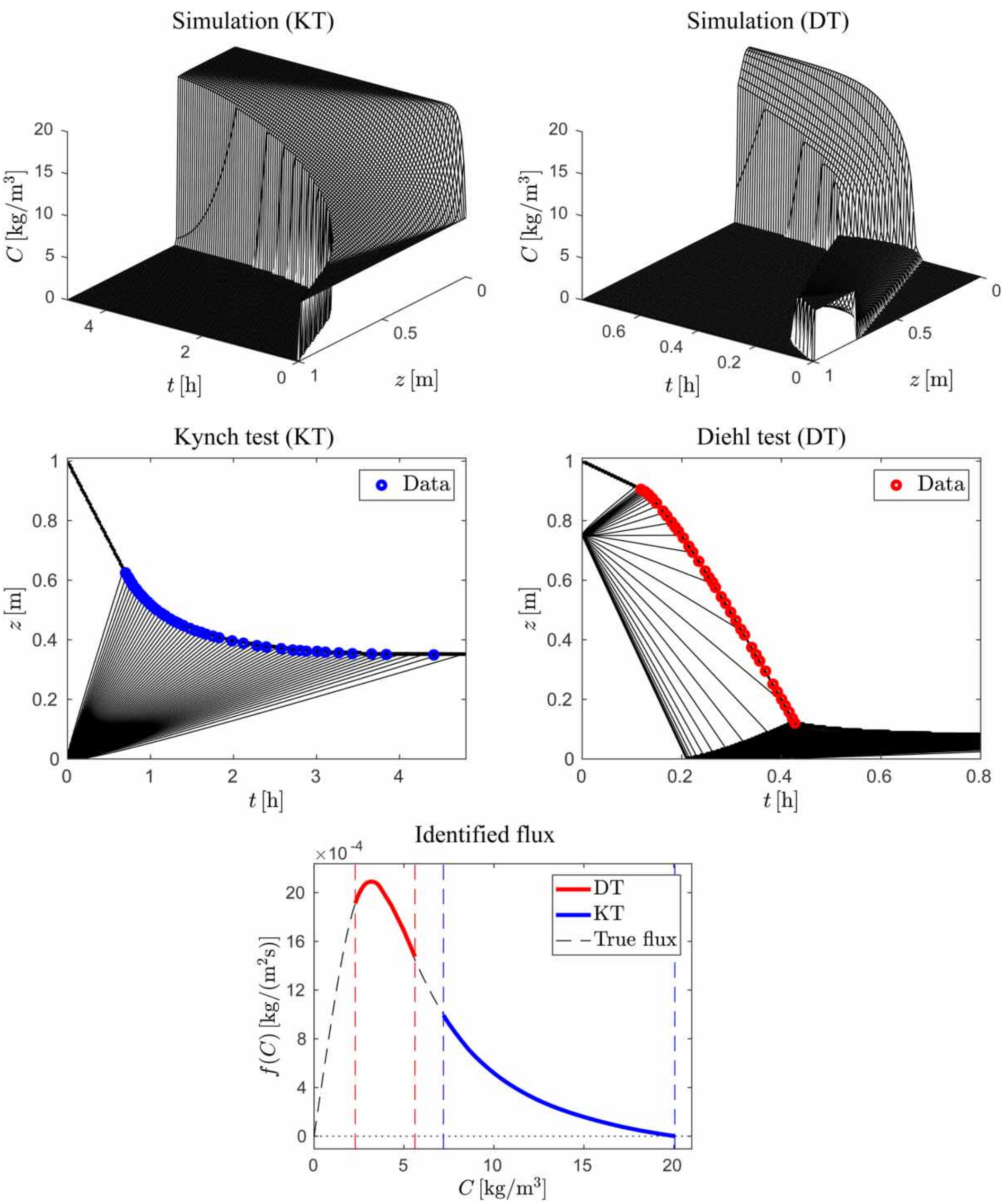

Figure 2 | Simulations of the Kynch test (KT) and Diehl test (DT) with the 'true' flux function shown as the dashed curve in the fifth subplot. The second row shows contours of the simulations in the first row. Method 2: The KT with initial concentration $C_0 = 7$ kg/m^3. Data points are taken from the curved convex part of the simulated SBL and the tail of the flux can be identified by (1), i.e., the interval $[C_0, C_{\max}]$. Method 3: The DT, where initially there is a layer of concentration $C_0 = 6$ kg/m^3 on top of clear water. Data points are taken from the curved concave part of the simulated SBL. The flux can be identified in an interval to the left of C_0 with formula (2).

equations; see Diehl (2015) for the full method. The flux can be identified from only one test; however, very special equipment and lots of data are required.

Method 5. Conical test (CT): One batch test with an initially homogeneous suspension of concentration C_0 is performed in a conical vessel with vertex at the bottom; see Figure 4. A large part of the flux can be identified by the parametric formula (Bürger *et al.* 2018a)

$$(C, f(C)) = \frac{H^3 C_0}{h(t)^2 (h(t) - t h'(t))} (1, \; -h'(t)), \qquad 0 \le t \le t_{\text{end}}, \tag{3}$$

where t_{end} is the time point when steady state is reached. The advantage of this method is that almost the entire flux

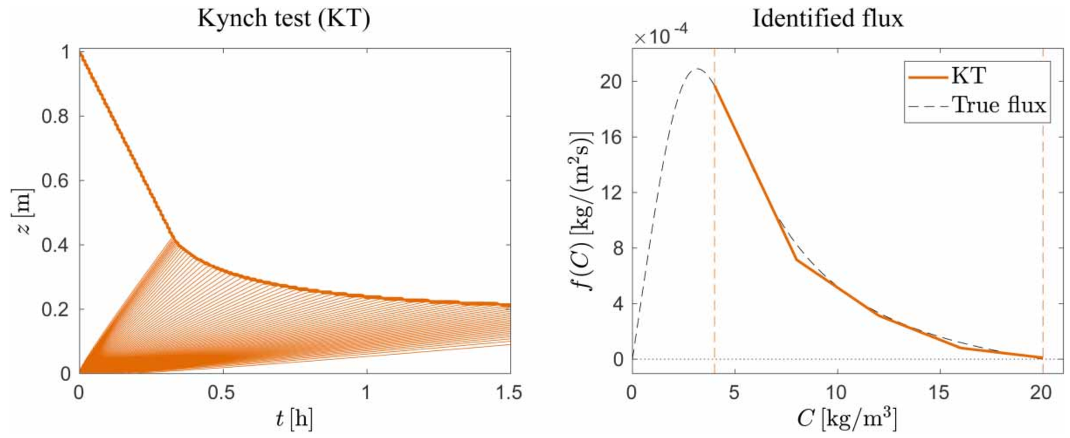

Figure 3 | Method 4: Simulation of a KT with $C_0 = 4$ kg/m^3 with 200^2 data points (z_i, t_j, C_{ij}), $i, j = 1, \ldots, 200$, which are all used for the flux identification with a finite-element method. Right: Identified flux function. The data contain no concentrations between 0 and 4 kg/m^3; hence the flux cannot be identified there.

can be estimated from only one test. While positive results are reported for some materials (Bürger *et al.* 2018b); different fluxes are estimated with CT and KT for other materials; see Celi (2018), who found that such differences increase with larger viscosity of the mixture. Wall friction effects and other two-dimensional phenomena influence a CT more than a KT.

Method 6. Rotational basket test (RBT) (Figure 4): The gravity force in a traditional batch test is replaced by a high centrifugal force. This means that the gravity-settling flux function, which we can write $f(C) = g\tilde{f}(C)$, where g is the gravity acceleration, is replaced by $r\omega^2\tilde{f}(C)$, where $r\omega^2$ is the centrifugal acceleration in a centrifugation force field at the distance r from the centre of rotation. Since the centrifugal acceleration varies with the radius, it is theoretically possible to estimate a large part of $\tilde{f}(C)$ (Careaga & Diehl 2020). This can be done with either a rotating tube ($\gamma = 0$) or a cylindrical basket ($\gamma = 1$) rotating with angular frequency ω around its axis of symmetry at $r = 0$. An approximate model PDE valid for $100\,\text{s}^{-1} \le \omega \le 1000\,\text{s}^{-1}$, which corresponds to 1,000–10 000 rpm, in cylindrical coordinates, is the following (Anestis & Schneider 1983; Bürger & Concha 2001):

$$\frac{\partial C}{\partial t} + \frac{1}{r^\gamma}\frac{\partial}{\partial r}(r^{1+\gamma}\omega^2\tilde{f}(C)) = 0, \qquad 0 \le r_0 < r < r_1,$$

where r_0 and r_1 are the inner and outer radii (top and bottom of the suspension), respectively. Contrary to gravity sedimentation, the concentration below the SBL decreases until waves from the bottom reach the SBL. At that time point, denoted by t_{end}, the curvature of the SBL changes; see Figure 6 (left), and the recording of $h(t)$ should be done up to t_{end}. If the concentration just below the SBL at t_{end} is C_{low}, then $\tilde{f}(C)$ can be identified in the interval $[C_{\text{low}}, C_0]$ given by the following formula (Careaga & Diehl 2020):

$$(C, \tilde{f}(C)) = C_0\left(\frac{r_0}{h(t)}\right)^{1+\gamma}\left(1, \frac{h'(t)}{\omega^2 h(t)}\right), \qquad 0 \le t \le t_{\text{end}} \qquad (4)$$

Once a part of $\tilde{f}(C)$ has been identified from an RBT, the corresponding part of the gravity-settling flux function is

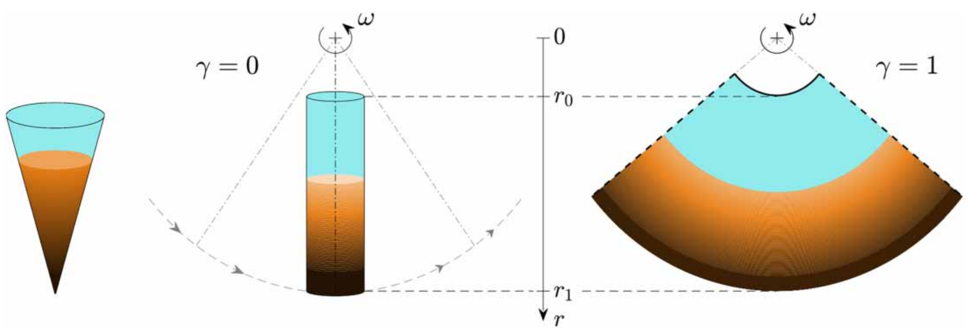

Figure 4 | Snapshots from a batch test in a cone (left) and in a centrifuge: tube (middle) and basket (right).

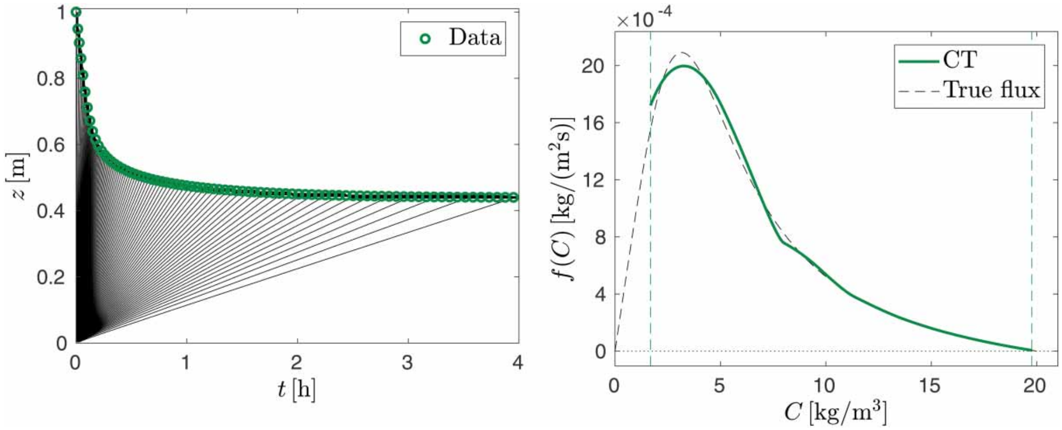

Figure 5 | Method 5: A batch test in a full conical vessel (with its vertex at the bottom) with initial concentration $C_0 = 1.7$ kg/m^3 are simulated. The flux function can be identified from C_0 up to the maximum concentration with formula (3).

$f(C) = g\tilde{f}(C)$. An advantage is that only one experiment is required and it is much faster than in all other methods. A disadvantage is that a centrifuge is needed.

DISCUSSION

All methods (except for Method 4) depend on accurate measurement of the SBL, to which a function $h(t)$ is fitted, see Supplementary Material, so that the derivative function $h'(t)$ is available. One property of Methods 2, 3, 5 and 6, where a part of the flux can be identified from only one experiment, is that a large variation of $h'(t)$, even in a small time interval, corresponds to a large portion of the identified flux function. Hence, it is important to have many data points in such time intervals. In Method 5 (CT), it is important to have many data points in the beginning of the test; see Figure 5, while in Method 6 (RBT), this is important at a later stage; see Figure 6. If compression of sludge occurs above a critical concentration, then the flux function cannot be identified above this concentration, except for Method 4, which has the possibility to identify the effective solids stress function simultaneously with the flux. Since the critical concentration is normally unknown, it is in several methods difficult to know when to stop the recording of the SBL. The RBT may then be advantageous, since the initial concentration C_0 is the upper endpoint of the interval of identification; hence, this should be chosen less than the critical one. Methods 5 (CT) and 6 (RBT) have the possibility to identify a larger portion of the flux function than the others.

After the graph of (a portion of) the flux function $f(C)$ has been obtained; either with piecewise straight lines in Method 4, or parametric formulas in the other methods, one usually wants to have a simple functional expression for the flux

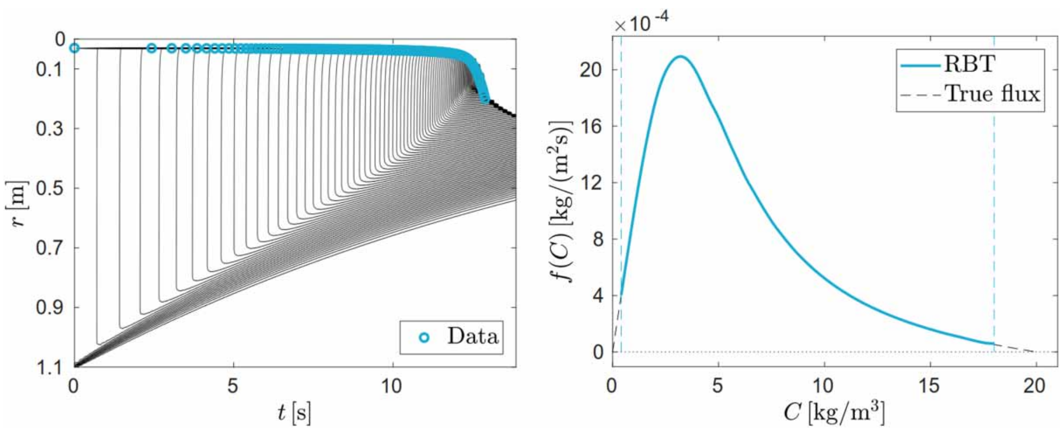

Figure 6 | Method 6: RBT (left) with initial concentration $C_0 = 18$ kg/m^3 and $r_0 = 0.03$ m are simulated for a rotational basket ($\gamma = 1$). The thin lines are iso-concentration curves. In centrifugal settling, the concentration below the SBL decreases with time until the SBL meets waves with high concentrations from the bottom. This occurs when the curvature of the SBL changes. The flux function can be identified from C_0 downwards with formula (4).

$f(C)$ to use in a simulation program. One possibility is to utilize explicit expressions that can be derived from the parametric formulas (1)–(4) by eliminating the time variable. To obtain a good fit of $h(t)$, one normally has to use several time subintervals of the experiment. If on each such subinterval $h(t)$ is represented by a cubic spline, then $f(C)$ is given by an explicit formula on each corresponding concentration interval. We refer to Bürger & Diehl (2013) and Bürger et al. (2018a) for all details. In addition to the fact that one does not obtain a simple formula for $f(C)$, another drawback of that approach is that the entire flux function is not identified so that the remaining parts have to be fitted with, for example, low-order polynomials. The other possibility is to use a nonlinear least-squares fit of one or a couple of simple expressions to the obtained graphs of $f(C)$ that the identification method has given.

Comments made here on experimental properties are supported by references and unpublished experience. A method that we have not yet investigated by means of PDE solutions is the one by Martin et al. (1995), who used fluidization. They used the balance of an upward fluid velocity and the settling velocity in a liquid fluidized bed to determine the settling velocity and thereby the flux function.

CONCLUSIONS

Based on PDE theory, there exist several possible methods to identify the hindered-settling flux function without prescribing any functional expression. The methods have been exemplified with synthetic data for comparison and illustration of how large an interval of concentration the flux function can be identified in. The traditional Kynch settling test (Method 1), which gives one point on the flux curve from each experiment, is heavily outscored by the other methods, which, at least theoretically, can estimate a large portion of the flux function from one or two experiments. All but one of those methods depend on the accurate measurement of the SBL, to which a function $h(t)$ is fitted, so that its derivative $h'(t)$ is easily obtained. Both these functions are then used in explicit formulas to obtain the graph of the flux function in an interval of concentrations. Of the methods reviewed, large such intervals can be obtained with the conical test (Method 5) and the rotational basket test (Method 6).

Our contribution is focussed on the theoretical properties of the identification methods. As for experimental conditions with real suspensions, many aspects are added that may imply that one method is preferable to another.

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SUPPLEMENTARY MATERIAL

The Supplementary Material for this paper is available online at https://dx.doi.org/10.2166/wst.2020.113.

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